

1 stepped pressure equilibrium code : descrp

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1.1 outline

1. Theoretical foundation, an introduction to the geometry and numerics, and compilation instructions.

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1.2 multi-region, relaxed MHD

The Stepped Pressure Equilibrium Code, SPEC, seeks numerical solutions to macroscopic force balance between the pressure and the magnetic field in arbitrary, non-axisymmetric toroidal configurations, with fields of arbitrary topology. Generally, non-axisymmetric toroidal magnetic fields are non-integrable. Accordingly, SPEC does not assume that the magnetic field is everywhere tangential to a set of continously nested magnetic surfaces.

The most elegant approaches for computing MHD equilibria begin with an energy principle. Our equilibrium model, which we call multi-region, relaxed MHD [1, 2], is based on a constrained energy principle that combines ideal MHD and Taylor relaxation theory [3] and is consistent with KAM theory [4, 5, 6]. Where the constraints of ideal MHD are applied, topological variations in the magnetic field are prohibited. Where these constraints are not applied, we assume, as did Taylor, that a weakly resistive plasma will relax to minimize the plasma energy subject to the constraint of conserved helicity. In these relaxed regions, reconnection phenomena are allowed, so that magnetic islands and field-line chaos may form. However, some flux surfaces with particularly irrational rotational-transform are expected to survive, and it is at these locations where pressure gradients are allowed.

Consider a plasma region [1] comprised of a set of N nested annular regions, which are separated by a discrete set of toroidal interfaces, \mathcal{I}_l . We insist that the fields are tangential to the interfaces. In each volume, \mathcal{V}_l , bounded by the \mathcal{I}_{l-1} and \mathcal{I}_l interfaces, the plasma energy, U_l , the global-helicity, H_l , and the mass/entropy, M_l , are given by the integrals:

$$U_l = \int_{\mathcal{V}_l} \left(\frac{p}{\gamma - 1} + \frac{B^2}{2\mu_0} \right) dv, \quad H_l = \int_{\mathcal{V}_l} \mathbf{A} \cdot \mathbf{B} dv, \quad M_l = \int_{\mathcal{V}_l} p^{1/\gamma} dv, \quad (1)$$

where $\mathbf{B} = \nabla \times \mathbf{A}$. The pressure, p , is a scalar function of position. The equilibrium states that we seek minimize the total plasma energy, subject to the constraints of conserved helicity and conserved mass/entropy in each annular region. The functional we seek to extremize is $F = \sum_l F_l$ where $F_l \equiv (U_l - \mu_l H_l/2 - \nu_l M_l)$, where μ_l and ν_l are Lagrange multipliers (and are constant over each volume).

We allow for arbitrary variations in (i) the pressure in each volume, δp , (ii) the magnetic field in each volume, $\delta \mathbf{A}$, and (iii) the geometry of the interfaces, $\boldsymbol{\xi}$; except that we assume the magnetic field remains tangential to the interfaces. At the interfaces, and only at the interfaces, the variation in the geometry and fields are constrained according to $\delta \mathbf{A} = \boldsymbol{\xi} \times \mathbf{B}$.

The first variation in F_l is given

$$\delta F_l = \int_{\mathcal{V}_l} \left(\frac{1}{\gamma - 1} - \frac{\nu_l p^{1/\gamma}}{\gamma p} \right) \delta p dv + \int_{\mathcal{V}_l} \left(\frac{\nabla \times \mathbf{B}}{\mu_0} - \mu_l \mathbf{B} \right) \cdot \delta \mathbf{A} dv + \int_{\partial \mathcal{V}_l} \left(\frac{p}{\gamma - 1} - \nu_l p^{1/\gamma} - \frac{B^2}{2\mu_0} \right) \boldsymbol{\xi} \cdot \mathbf{n} ds \quad (2)$$

The Euler–Lagrange equations show that plasma states that extremize F satisfy the following: (i) in each annulus the pressure obeys $\nu_l p^{1/\gamma} = \gamma p/(\gamma - 1)$, i.e. the pressure is constant. (ii) in each annulus, the magnetic field is a linear, force-free “Beltrami” field given by $\nabla \times \mathbf{B}_l = \mu_l \mathbf{B}_l$; and, by using the Euler–Lagrange equation for the pressure, (iii) the *total* pressure is continuous across the ideal interfaces, $[[p + B^2/2]] = 0$.

Nontrivial pressure profiles are supported by the ideal interfaces, across which a pressure discontinuity is allowed provided there is a compensating discontinuity in the tangential field. The equilibrium solutions are topologically-constrained but partially-relaxed *stepped-pressure* states that we call multi-region, relaxed MHD equilibria. (Topological constraints on magnetic

reconnection have been observed in a similar context [7].) An analysis of the force-balance condition, $[[p + B^2/2]] = 0$, shows that, generally, in order for an interface to support pressure, it must have irrational rotational-transform [8].

At first, the restriction to stepped-pressure profiles seems artificial. However, an equilibrium state with a nontrivial, *continuous* pressure that satisfies $\mathbf{B} \cdot \nabla p = 0$ with a nonintegrable (partially chaotic) magnetic field *must* have an *uncountable* infinity of discontinuities in the pressure gradient. Standard numerical discretizations, e.g. finite differences, for constructing solutions to $\nabla p = \mathbf{j} \times \mathbf{B}$ with continuous, nontrivial pressure profiles and nonintegrable fields will not produce reliable convergence, as the solution being approximated has structure on all scales.

In contrast, the multi-region relaxed MHD approach described above is based on an energy integral. This only requires that the pressure be an integrable function and does not require differentiability. Specifying the profiles discretely, rather than continuously, is a practical means of retaining some control over the pressure and transform profiles while making minimal assumptions regarding the topology of the field: it is only assumed that at least some flux surfaces exist, and that pressure gradients coincide with flux surfaces with strongly irrational transform. A strong motivation for adopting this model is that Bruno & Laurence [9] have proved that, under certain conditions, 3D stepped-pressure equilibria exist, thus putting the MRXMHD model on a strong mathematical foundation. Arbitrarily many interfaces may be included, so any pressure profile may be approximated arbitrarily closely.

A fixed-boundary equilibrium is defined by (i) the shape of the outer boundary, (ii) the pressure as a function of toroidal flux, e.g. $p(\psi_t) = p_l$ for $\psi_t \in [\psi_{t,l-1}, \psi_{t,l}]$, and (iii) the rotational-transform of the interfaces. An initial “guess” for the geometry of the internal interfaces is required. SPEC uses a Fourier representation in the poloidal and toroidal angles, and a high-order polynomial finite element basis functions in the radial coordinate to describe the magnetic vector potential. Differentiating the constrained energy functional with respect to the numerical degrees of freedom in the vector potential gives rise to a set of sparse linear equations that define the Beltrami fields in each volume, and the construction of Beltrami fields is trivially distributed over multiple cpus. Standard numerical methods, e.g. multi-dimensional Newton’s method, are then used to vary the internal interface geometry in order to locate an extremum of the constrained energy functional, i.e. to solve for force balance across the interfaces.

1.2.1 some additional mathematical details

The functional we seek to extremize is

$$F = \sum_{l=1}^{N_V} (U_l - \mu_l H_l / 2 - \nu_l M_l), \quad (3)$$

where μ_l and ν_l are Lagrange multipliers (and are constant over each volume, \mathcal{V}_l). The first variation in the plasma energy, allowing variations in the pressure, δp , the field, $\delta \mathbf{A}$, and interface geometry, $\boldsymbol{\xi}$, is given

$$\delta U_l = \int_{\mathcal{V}_l} \left(\frac{\delta p}{\gamma - 1} + \frac{\mathbf{B} \cdot \nabla \times \delta \mathbf{A}}{\mu_0} \right) dv + \int_{\partial \mathcal{V}_l} \left(\frac{p}{\gamma - 1} + \frac{B^2}{2\mu_0} \right) (\mathbf{n} \cdot \boldsymbol{\xi}) ds, \quad (4)$$

Using the identity $\nabla \cdot (\mathbf{A} \times \mathbf{B}) = \mathbf{B} \cdot \nabla \times \mathbf{A} - \mathbf{A} \cdot \nabla \times \mathbf{B}$ and integrating by parts we obtain

$$\delta U_l = \int_{\mathcal{V}_l} \left(\frac{\delta p}{\gamma - 1} + \frac{\delta \mathbf{A} \cdot \nabla \times \mathbf{B}}{\mu_0} \right) dv + \int_{\partial \mathcal{V}_l} \left(\frac{p}{\gamma - 1} + \frac{B^2}{2\mu_0} \right) (\mathbf{n} \cdot \boldsymbol{\xi}) ds + \int_{\partial \mathcal{V}_l} \frac{\mathbf{n} \cdot \delta \mathbf{A} \times \mathbf{B}}{\mu_0} ds. \quad (5)$$

The interfaces are assumed to be ideal, so in the surface integrals we make use of Faraday’s law $\partial_t \mathbf{B} = \nabla \times \mathbf{E}$ and the ideal Ohm’s law $\mathbf{E} + \mathbf{v} \times \mathbf{B} = 0$ to obtain the expression $\delta \mathbf{A} = \boldsymbol{\xi} \times \mathbf{B}$. The variation in the plasma energy becomes

$$\delta U_l = \int_{\mathcal{V}_l} \left(\frac{\delta p}{\gamma - 1} + \frac{\delta \mathbf{A} \cdot \nabla \times \mathbf{B}}{\mu_0} \right) dv + \int_{\partial \mathcal{V}_l} \left(\frac{p}{\gamma - 1} - \frac{B^2}{2\mu_0} \right) (\mathbf{n} \cdot \boldsymbol{\xi}) ds. \quad (6)$$

A similar analysis shows that the first variation in the helicity is

$$\delta H_l = 2 \int_{\mathcal{V}_l} \mathbf{B} \cdot \delta \mathbf{A} dv. \quad (7)$$

The variation in the plasma mass is

$$\delta M_l = \int_{\mathcal{V}_l} \frac{p^{1/\gamma}}{\gamma p} \delta p dv + \int_{\partial \mathcal{V}_l} p^{1/\gamma} (\mathbf{n} \cdot \boldsymbol{\xi}) ds.$$

Only the variations in the geometry normal to the interfaces, $(\mathbf{n} \cdot \boldsymbol{\xi})$, are relevant: tangential variations do not alter the energy functional. To constrain the tangential degrees of freedom, additional constraints derived from minimizing the spectral width are included.

1.3 Description of geometry and numerical methods

The code can operate in Cartesian, cylindrical or toroidal geometry. In each case, stellarator symmetry may or may not be enforced (under construction). The vector potential is discretized using finite-elements in the radial direction, and Fourier harmonics in the poloidal and toroidal angles.

1.3.1 Cartesian, cylindrical, or toroidal geometry

The code uses (s, θ, ζ) as the internal coordinates, which may represent Cartesian, cylindrical or toroidal coordinates as follows.

0. For Cartesian, we identify $\mathbf{x} = \theta \hat{\mathbf{i}} + \zeta \hat{\mathbf{j}} + Z(s, \theta, \zeta) \hat{\mathbf{k}}$, where $\hat{\mathbf{i}}, \hat{\mathbf{j}}$ and $\hat{\mathbf{k}}$ are the standard Cartesian basis vectors.
1. For cylindrical, we identify $\mathbf{x} = R(s, \theta, \zeta) \hat{\mathbf{r}} + \zeta \hat{\mathbf{k}}$, where $\hat{\mathbf{r}} \equiv \cos \theta \hat{\mathbf{i}} + \sin \theta \hat{\mathbf{j}}$.
2. For toroidal, we identify $\mathbf{x} = R(s, \theta, \zeta) \hat{\mathbf{R}} + Z(s, \theta, \zeta) \hat{\mathbf{k}}$, where $\hat{\mathbf{R}} \equiv \cos \zeta \hat{\mathbf{i}} + \sin \zeta \hat{\mathbf{j}}$.

Note that in the toroidal case, the poloidal angle, θ , is arbitrary.

A set of $l = 1, N_V$ nested, toroidal surfaces is assumed given. For expedience, we restrict attention to stellarator symmetric devices [10] so that the interfaces may be described

$$\begin{aligned} R_l(\theta, \zeta) &= \sum_j R_{l,j} \cos(m_j \theta - n_j \zeta), \\ Z_l(\theta, \zeta) &= \sum_j Z_{l,j} \sin(m_j \theta - n_j \zeta). \end{aligned} \quad (8)$$

The coordinate functions $R(s, \theta, \zeta)$ and $Z(s, \theta, \zeta)$ take the form

$$\begin{aligned} R(s, \theta, \zeta) &= \sum_j R_j(s) \cos(m_j \theta - n_j \zeta), \\ Z(s, \theta, \zeta) &= \sum_j Z_j(s) \sin(m_j \theta - n_j \zeta), \end{aligned} \quad (9)$$

where the functions $R_j(s)$, $Z_j(s)$ are constructed by piecewise-cubic interpolation of the $R_{l,j}$ and $Z_{l,j}$. In the l -th annulus, bounded by the $(l-1)$ -th and l -th interfaces, a general covariant representation of the magnetic vector-potential is written

$$\bar{\mathbf{A}}_l = \bar{A}_{s,l} \nabla s + \bar{A}_{\theta,l} \nabla \theta + \bar{A}_{\zeta,l} \nabla \zeta. \quad (10)$$

To this add $\nabla g_l(s, \theta, \zeta)$, where g_l satisfies

$$\begin{aligned} \partial_s g_l(s, \theta, \zeta) &= -\bar{A}_{s,l}(s, \theta, \zeta), \\ \partial_\theta g_l(s_{l-1}, \theta, \zeta) &= -\bar{A}_{\theta,l}(s_{l-1}, \theta, \zeta) + \psi_{t,l-1}, \\ \partial_\zeta g_l(s_{l-1}, 0, \zeta) &= -\bar{A}_{\zeta,l}(s_{l-1}, 0, \zeta) + \psi_{p,l-1}, \end{aligned} \quad (11)$$

for arbitrary constants $\psi_{t,l-1}$, $\psi_{p,l-1}$, which are the toroidal and poloidal-fluxes on the interior of surface $l-1$. Then $\mathbf{A}_l = \bar{\mathbf{A}}_l + \nabla g_l$ is given by $\mathbf{A}_l = A_{\theta,l} \nabla \theta + A_{\zeta,l} \nabla \zeta$ with

$$\begin{aligned} A_{\theta,l}(s_{l-1}, \theta, \zeta) &= \psi_{t,l-1}, \\ A_{\zeta,l}(s_{l-1}, 0, \zeta) &= \psi_{p,l-1}. \end{aligned} \quad (12)$$

This specifies the gauge. For stellarator symmetric equilibria, $A_{\theta,l}$ and $A_{\zeta,l}$ may be represented by cosine series

$$\begin{aligned} A_{\theta,l}(s, \theta, \zeta) &= \sum_j A_{\theta,l,j}(s) \cos(m_j \theta - n_j \zeta), \\ A_{\zeta,l}(s, \theta, \zeta) &= \sum_j A_{\zeta,l,j}(s) \cos(m_j \theta - n_j \zeta), \end{aligned} \quad (13)$$

where $A_{\theta,l,j}(s)$ and $A_{\zeta,l,j}(s)$ are represented using finite-elements.

1.4 Compilation instructions

1. The source is kept under CVS: `>cvs -d /u/shudson/cvs_Spec/ checkout Spec`
2. Compilation is provided by a Makefile: `>make xspec`. Try `>make help` for compilation options.
 - (a) The compilation flags are given by **FLAGS**. These may be over-ruled by command line arguments.
 - (b) Compilation flags must be set that convert single precision to double precision, e.g. `make FLAGS="--dbl"`.
 - (c) The NAG library is used and must be correctly linked.
 - (d) To apply a patch: `>patch -p1 < file`

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